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Arsenate Surface Speciation at the Hematite-Water Interface

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Beamline(s): X11A

Introduction: Arsenate (As(V)) is a ubiquitous toxic metalloid in oxic terrestrial/aquatic environments due to indigenous and anthropogenic inputs. In order to accurately predict the transport of As(V) in subsurface environments, detailed mechanistic information (i.e., stoichiometric reactions and surface complexes) is needed to better understand As(V) reactions at soil mineral-water interfaces. In this study, we investigated As(V) coordination environments at the hematite-water interface as a function of pH and loading level using in-situ Extended X-ray Absorption Fine Structure spectroscopy (EXAFS).

Methods and Materials: Synthetic hematite [1] was reacted with sodium arsenate solution at pH 4-8 using a batch adsorption method (4-8 g L^{-1} and $[As(V)]_o$ = 0.45-1.5 mmol)[2]. In-situ EXAFS analyses were performed on As(V) reacted hematite paste.

Results: EXAFS analysis on the As(V) sorption samples revealed two As-Fe distances of ~2.8 and ~3.3 angstroms at a loading level 855-2225 mg m^{-2} at pH 4.5 and 8 (Fig.1). Based on the theoretical molecular configuration of adsorbed arsenate on hematite surfaces (Fig.2), two different inner-sphere complexes (i.e., bidentate binuclear and bidentate mononuclear complexes) on edge-sharing and face-sharing iron octahedral sites are suggested.

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References:

[1]. U. Schwertmann and R.M. Cornell. Iron Oxides in the Laboratory: Preparation and Characterization. VCH, Weinheim/New York, 1991. p. 102.

[2].Y. Arai, E.J. Elzinga, and D.L. Sparks. “X-ray absorption spectroscopic investigation of arsenite and arsenate adsorption at the aluminum oxide-water interface”. Journal of Colloid and Interface Science. 235. 80-88. (2001)

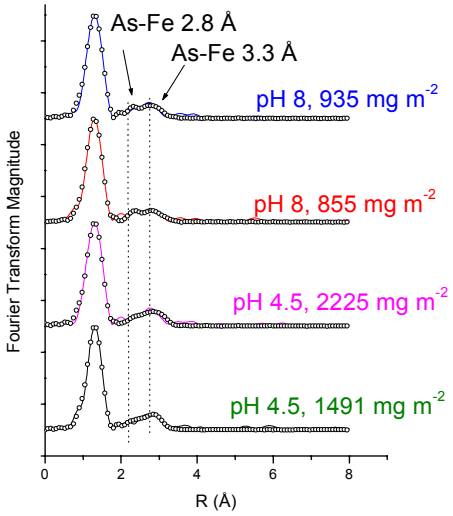

Fig.-1: Least-square fit to Fourier transforms of arsenate adsorbed on hematite.

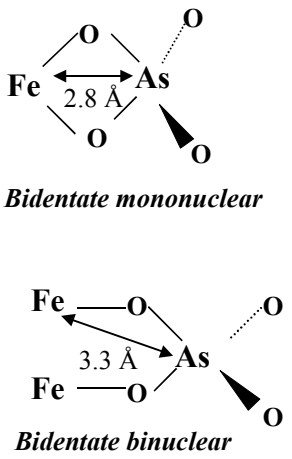

Fig.-2: Theoretical molecular configuration of adsorbed arsenate on hematite surfaces.